International Tables for Crystallography (2006). Vol. D, Section 3.3.8.3, pp. 418–419.

Table 3.3.8.1. *Lattice planes (hkl) and lattice rows [uvw] that are mutually perpendicular (after Koch, 1999)*

Lattice	Lattice plane (*hkl*)	Lattice row [*uvw*]	Perpendicularity condition and quantity $j' = hu + kv + lw$
Triclinic	–	–	–
Monoclinic (unique axis *b*)	(010)	[010]	–
Monoclinic (unique axis *c*)	(001)	[001]	–
Orthorhombic	(100) (010) (001)	[100] [010] [001]	– – –
Hexagonal and rhombohedral (hexagonal axes)	(*hki*0) (0001)	[*uv*0] [001]	$u = 2h + k,\ v = h + 2k,\ j' = 2h^2 + 2k^2 + 2hk$ –
Rhombohedral (rhombohedral axes)	$(h, k, -h-k)$ (111)	$[u, v, -u-v]$ [111]	$u = h,\ v = k,\ j' = 2h^2 + 2k^2 + 2hk$ –
Tetragonal	(*hk*0) (001)	[*uv*0] [001]	$u = h,\ v = k,\ j' = h^2 + k^2$ –
Cubic	(*hkl*)	[*uvw*]	$u = h,\ v = k,\ w = l;\ j' = h^2 + k^2 + l^2$

$$j' = hu + kv + lw \quad (\text{scalar product } \mathbf{r}^{\star}_{hkl} \cdot \mathbf{t}_{uvw})$$

with sublattice index

$$[j] = |j'| \text{ for } j' = 2n + 1$$
$$= |j'|/2 \text{ for } j' = 2n.$$

Here, the indices of the plane (*hkl*) and of the perpendicular row [*uvw*] are referred to a primitive lattice basis (primitive cell). For centred lattices, described by conventional bases, modifications are required; these and further examples are given by Koch (1999). Formulae and tables are presented by Friedel (1926, pp. 245–252) and by Donnay & Donnay (1972). The various equations for the quantity j' are also listed in the last column of Table 3.3.8.1.

Note that in the tetragonal system for any (*hk*0) reflection twin and any [*uv*0] twofold rotation twin, the coincidence lattices are also tetragonal and have the same lattice parameter *c*. Further details are given by Grimmer (2003). An analogous relation applies to the hexagonal crystal family for (*hki*0) and [*uv*0] twins. In the cubic system, the following types of twin lattices occur:

(111) and [111] twins: hexagonal *P* lattice (*e.g.* spinel twins);
(*hk*0) and [*uv*0] twins: tetragonal lattice;
(*hhl*) and [*uuw*] twins: orthorhombic lattice;
(*hkl*) and [*uvw*] twins: monoclinic lattice.

Note that triclinic twin lattices are not possible for a cubic lattice.

After these general considerations of coincidence-site and twin lattices and their lattice index, specific cases of 'triperiodic twins' are treated in Section 3.3.8.3. In addition to the characterization of the twin lattice by its index [*j*], the Σ notation used in metallurgy is included.

3.3.8.3. *Twins with three-dimensional twin lattices ('triperiodic' twins)*

The following cases of exact superposition are distinguished:

(i) *Twins with* $[j] = 1$ ($\Sigma 1$ *twins*). Here, the crystal lattice and the twin lattice are identical, *i.e.* the coincidence (parallelism) of the two oriented crystal lattices is complete. Hence, any twin operation must be a symmetry operation of the point group of the lattice (holohedry), but not of the point group of the crystal. Consequently, this twinning can occur in 'merohedral' point groups only. This *twinning by merohedry* (*parallel-lattice twins*, *twins with parallel axes*) will be treated extensively in Section 3.3.9.

(ii) *Twins with* $[j] = 2$ ($\Sigma 2$ *twins*). This twinning does not occur systematically among the cases listed in Table 3.3.8.1, except for special metrical relations. Example: a primitive orthorhombic lattice with $b/a = \sqrt{3}$ and twin reflection plane (110) or ($\bar{1}$10). The coincidence lattice is hexagonal with $a_{\rm hex} = 2a$ and $[j] = 2$.

(iii) *Twins with* $[j] = 3$ ($\Sigma 3$ *twins*). Twins with $[j] = 3$ are very common among rhombohedral and cubic crystals ('spinel law') with the following two representative twin operations:

(*a*) twofold rotation around a threefold symmetry axis [111] (cubic or rhombohedral coordinate axes) or [001] (hexagonal axes);

(*b*) reflection across the plane (111) or (0001) normal to a threefold symmetry axis.

Both twin operations belong to the same twin law if the crystal is centrosymmetric. Well known examples are the (0001) contact twins of calcite, the penetration twins of iron borate, $FeBO_3$, with the calcite structure, and the spinel twins of cubic crystals (*cf.* Examples 3.3.6.5, 3.3.6.6 and Figs. 3.3.6.4–3.3.6.6). For crystals with a rhombohedral (*R*) lattice, the coincidence lattice is the primitive hexagonal (*P*) sublattice (whose unit cell is commonly used for the hexagonal description of rhombohedral crystals). Here, the two centring points inside the triple hexagonal *R* cell do not belong to the coincidence sublattice which is, hence, of index $[j] = 3$. The same holds for the spinel twins of cubic crystals, provided only one of the four threefold axes is involved in the twinning.

(iv) *Twins with* $[j] > 3$ ($\Sigma > 3$ *twins*). Whereas twins with $[j] = 3$ are very common and of high importance among minerals and metals, twins with higher lattice indices occur hardly at all. All these 'high-index' twins can occur systematically only in tetragonal, hexagonal, rhombohedral and cubic crystals, due to the geometric perpendicularity relations set out in Table 3.3.8.1. Note that for special lattice metrics (axial ratios and angles) they can occur, of course, in any crystal system. These special metrics, however, are not enforced by the crystal symmetry and hence the coincidences are not strict, but only 'pseudo-coincidences'.

Examples

(1) Tetragonal twins with twin reflection planes {210} or {130}, or twofold twin axes ⟨210⟩ or ⟨130⟩ lead to $[j] = 5$, the largest value of [*j*] that has been found so far for tetragonal twins. The coincidence lattice is again tetragonal with $\mathbf{a}' = 2\mathbf{a} + \mathbf{b}$, $\mathbf{b}' = -\mathbf{a} + 2\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$ and is shown in Fig. 3.3.8.1. An actual example, $SmS_{1.9}$ (Tamazyan *et al.*, 2000*b*), is discussed in Section 3.3.9.2.4.

(2) There exist several old and still unsubstantiated indications for a $[j] = 5$ *cubic garnet twin* with twin reflection plane (210), *cf.* Arzruni (1887); Tschermak & Becke (1915, p. 594).

(3) *Klockmannite, CuSe* (Taylor & Underwood, 1960; Takeda & Donnay, 1965). This hexagonal mineral seems to be the only example for a hexagonal twin with $[j] > 3$. X-ray diffraction experiments indicate a reflection twin on (13$\bar{4}$0), corresponding

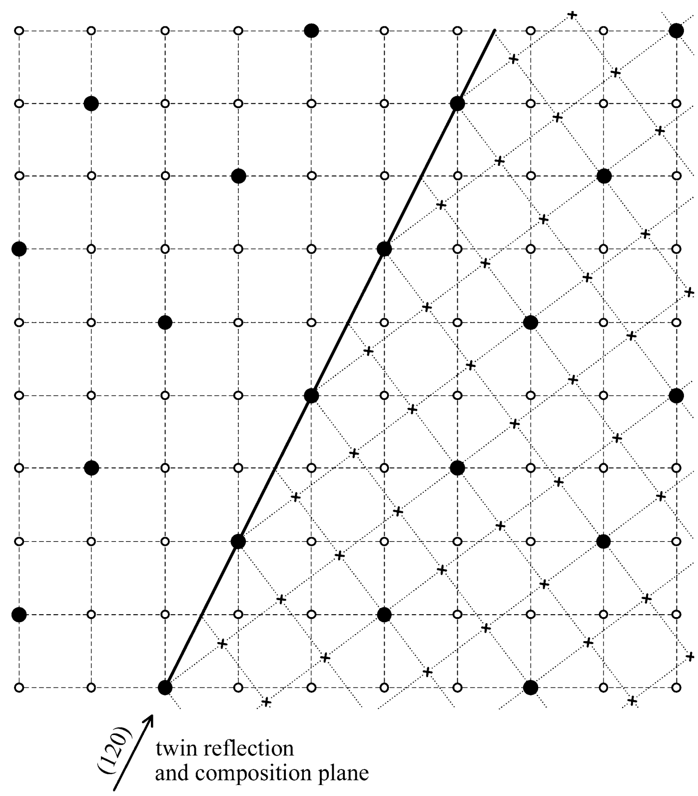

Fig. 3.3.8.1. Lattice relations of Σ5 twins of tetragonal crystals with primitive lattice: twin mirror plane and composition plane (120) with twin displacement vector **t = 0**. Small dots: lattice points of domain 1; small x: lattice points of domain 2; large black dots: Σ5 coincidence lattice.

to [*j*] = 13. Later structural studies, however, suggest the possibility of disorder instead of twinning.

(4) *Galena, PbS* (NaCl structure). Galena crystals from various localities often exhibit lamellae parallel to the planes {441} which are interpreted as (441) reflection twins with [*j*] = 33 (Σ33 twin) (*cf.* Niggli, 1926, Fig. 9k on p. 53). These natural twins are deformation and not growth twins. In laboratory deformation experiments, however, these twins could not be generated. A detailed analysis of twinning in PbS with respect to plastic deformation is given by Seifert (1928).

(5) For cubic metals and alloys *annealing twins* (*recrystallization twins*) with [*j*] > 3 are common. Among them *high-order twins* (*high-generation twins*) are particularly frequent. They are based on the Σ3 (spinel) twins (first generation) which may coalesce and form 'new twins' with $\Sigma9 = 3^2$ [second generation, with twin reflection plane (221)], $\Sigma27 = 3^3$ [third generation, twin reflection plane (115)], $\Sigma81 = 3^4$ [fourth generation, twin reflection plane (447)] *etc.* Every step to a higher generation increases Σ by a factor of three (Gottstein, 1984). An interesting and actual example is the artificial silicon *tricrystal* shown in Fig. 3.3.8.2, which contains three components related by two (111) reflection planes (first generation, two Σ3 boundaries) and one (221) reflection plane (second generation, one Σ9 boundary).

(6) The same type of tricrystal has been found in cubic magnetite (Fe_3O_4) nanocrystals grown from the biogenic action of magnetotactic bacteria in an aquatic environment (Devouard *et al.*, 1998). Here, HRTEM micrographs (Fig. 6 of the paper) show the same triple-twin arrangement as in the Si tricrystal above. The authors illustrate this triple twin by (111) spinel-type intergrowth of three octahedra exhibiting two Σ3 and one Σ9 domain pairs. The two Σ3 interfaces are (111) twin reflection planes, whereas the Σ9 boundary is very irregular and not a compatible planar (221) interface (*i.e.* not a twin reflection plane).

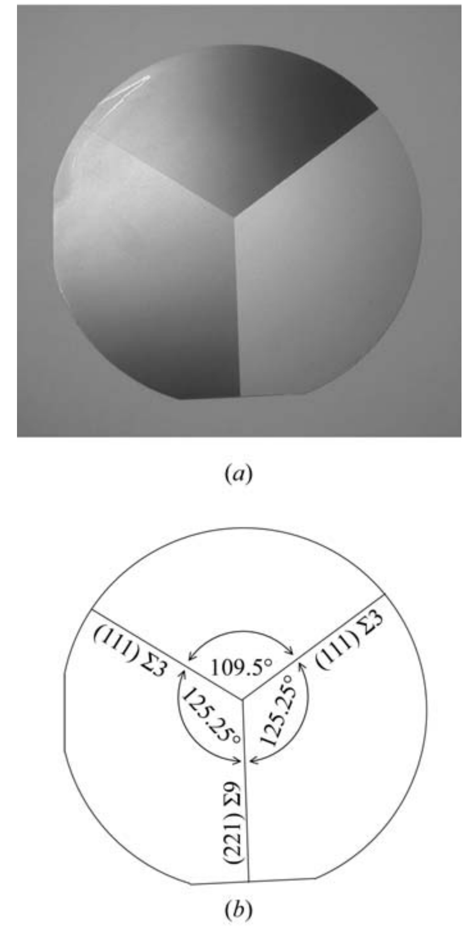

Fig. 3.3.8.2. (*a*) A (110) silicon slice (10 cm diameter, 0.3 mm thick), cut from a Czochralski-grown tricrystal for solar-cell applications. As seed crystal, a cylinder of three coalesced Si single-crystal sectors in (111) and (221) reflection-twin positions was used. Pulling direction [110] (Courtesy of M. Krühler, Siemens AG, München). (*b*) Sketch of the tricystal wafer showing the twin relations [twin laws *m*(111) and *m*(221)] and the Σ characters of the three domain pairs. The atomic structures of these (111) and (221) twin boundaries are discussed by Kohn (1956, 1958), Hornstra (1959, 1960) and Queisser (1963).

(7) A third instructive example is provided by the fivefold cyclic 'cozonal' twins (zone axis $[1\bar{1}0]$) of Ge nanocrystals (Neumann *et al.*, 1996; Hofmeister, 1998), which are treated in Section 3.3.10.6.5 and Fig. 3.3.10.11. All five boundaries between neighbouring domains (sector angles 70.5°) are of the Σ3(111) type. Second nearest (2 × 70.5°), third nearest (3 × 70.5°) and fourth nearest (4 × 70.5°) neighbours exhibit Σ9, Σ27 and Σ81 coincidence relations (second, third and fourth Σ generation), respectively, as introduced above in (5). These relations can be described by the 'cozonal' twin reflection planes (111), (221), (115) and (447). Since 5 × 70.5° = 352.5°, an angular gap of 7.5° would result. In actual crystals this gap is compensated by stacking faults as shown in Fig. 3.3.10.11. A detailed treatment of all these cases, including structural models of the interfaces, is given by Neumann *et al.* (1996).

(8) Examples of (hypothetical) twins with [*j*] > 1 due to metrical specialization of the lattice are presented by Koch (1999).

3.3.8.4. *Approximate (pseudo-)coincidences of two or more lattices*

In part (iv) of Section 3.3.8.2, three-dimensional lattice coincidences and twin lattices (sublattices) were considered under two restrictions:

(*a*) the lattice coincidences (according to the twin lattice index [*j*]) are *exact* (not approximate);